12

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EFFICIENCY STUDY OF IMPLICIT AND EXPLICIT TIME INTEGRATION OPERATORS FOR FINITE ELEMENT APPLICATIONS

by Michael G. Katona, Robert Thompson, and Jim Smith

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Direct integration techniques (step-by-step) are widely used for the time integration of discretized equations of motion that result from applying numerical techniques such as the finite element method to structural dynamic problems. The integration methods are commonly classified in two groups: (1) explicit methods, which are computationally fast per step but are limited to relatively small time steps due to numerical instability, and (2) implicit methods, which are computationally slower per step but are often capable of utilizing

Next page →

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significantly larger time steps with comparable accuracy. In many, if not most, problems it is not obvious which integration method is more efficient. In this study the Newmark Beta-Method is examined for stability, accuracy, and efficiency, wherein Beta = 0 provides an explicit algorithm, while Beta ≠ 0 provides an implicit algorithm. Both algorithms are used in the same finite element program to solve a soil-structure boundary value problem composed of a cylindrical steel shell encased in a relatively soft rock-like material and subjected to a surface blast loading. For this problem with linear system properties, the implicit method was significantly more efficient as measured by computer time. For nonlinear systems, the two methods are approximately equivalent in efficiency. A combined explicit-implicit integration technique is proposed for these types of interaction problems with two or more materials. The combined explicit-implicit algorithm employs explicit integration in the soft material and implicit integration in the stiff material with a potential increase in efficiency by an order of magnitude over either method applied individually.

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Direct integration techniques (step-by-step) are widely used for the time integration of discretized equations of motion that result from applying numerical techniques such as the finite element method to structural dynamic problems. In this study, the Newmark Beta-Method is examined for stability, accuracy, and efficiency, wherein Beta = 0 provides an explicit algorithm, while Beta ≠ 0 provides an implicit algorithm. Both algorithms are used in the same finite element program to solve a soil-structure boundary value problem composed of a cylindrical steel sheel encased in a relatively soft rock-like material and subjected to a surface blast loading. The implicit method was significantly more efficient as measured by computer time. For nonlinear systems, the two methods were approximately equivalent in efficiency. A combined explicit-implicit integration technique is proposed that employs explicit integration in the soft material and implicit integration in the stiff material with a potential increase in efficiency by an order of magnitude over either method applied individually.

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CONTENTS

INTRODUCTION

In the past two decades the finite element method has been widely used for solving structural dynamics problems. The numerical approximations inherent in the finite element technique include two broad categories: (a) spatial discretization and (2) temporal discretization. The former category deals with the approximation errors and efficiency of the assumed spatial distribution of the primary variables (e.g., displacement field), while the latter category deals with the approximation errors and efficiency involved with the time integration of the discretized equations of motion. In this study only the latter category is pursued and the discussion is restricted to direct integration methods (i.e., step-by-step). Other methods of solving the equations of motion such as eigenvalue analysis or method of characteristics are not considered because of their limitations for nonlinear problems.

Direct integration schemes are generally classified in two groups: implicit methods and explicit methods. This report examines these two methods in the light of numerical stability, accuracy, and efficiency for a class of problems,* characterized by a cylindrical structural liner embedded in a homogeneous rock-like material and subjected to a surface blast loading [1, 2].

Background

Numerous implicit and explicit integration operators are in current use and have been reported extensively in engineering literature. Some of the more popular implicit integration schemes are: the Newmark β-method ($\beta \neq 0$) [3], the Houbolt method [4], and the Wilson θ-method [5]. Explicit schemes are more commonly referred to by a finite difference operator such as the second central difference scheme [6]. Note the Newmark β-method with $\beta = 0$ is equivalent to the second central difference scheme and is an explicit method.

The fundamental difference between an explicit and implicit integration scheme is that in the explicit case the displacement vector for the current time step can be predicted directly from the known displacements, velocities, and accelerations of the previous time steps, whereas in the implicit case the current displacements are related to current accelerations (and possibly current velocities) as well as responses from previous time steps. As a result, the solution algorithm for the implicit scheme requires assembling a global mass and stiffness matrix into a set of coupled algebraic equations and solving the system by some technique such as Gaussian elimination.

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*Of current interest to the Defense Nuclear Agency (DNA).

On the other hand, the explicit algorithm only requires assembling the mass matrix and solving for the current acceleration. The restoring force vector (stiffness matrix times predicted displacement vector) is formed on the right-hand side at the element level, thereby eliminating the need of assembling the global stiffness matrix. If a lumped mass procedure is used (as is generally done), the accelerations are uncoupled and can be computed rapidly.

The trade-off one pays for the rapid explicit algorithm is the requirement of a small time step to avoid numerical instability. When instability occurs the computed responses become wildly erratic, oscillating many orders of magnitude. Numerical instability is governed by the frequency content of the discretized system and will be discussed later.

The potential advantage of some implicit integration schemes is that they are unconditionally stable, allowing a much larger time step controlled by integration accuracy (as opposed to integration stability).

In short, if computational efficiency is measured by the computer cost (time) to accurately integrate the equations of motion over a given time range of interest, then the explicit method has the advantage of rapid solutions per time step but the disadvantage of requiring many time steps. The reverse is true for the implicit method.

It cannot be categorically claimed that one method is more efficient than the other. Rather, the question of efficiency is highly problem dependent, involving such factors as: finite element mesh topology, types of elements, loading function, material properties, degree of nonlinearity, method of characterizing mass matrix, and the size of the system. Discussion of these influences are given in References 7 and 8.

Recently the idea has been advanced to simultaneously employ implicit and explicit integration operators over different regions of the finite element mesh to take optimum advantage of each method. The above notion, as well as explicit versus implicit efficiency studies, is pursued in the course of this investigation.

Objective and Scope

This investigation is restricted to the family of integration operators contained in Newmark's β-method [3] wherein $\beta = 0$ provides an explicit scheme and $\beta \neq 0$ provides an implicit scheme. The test boundary value problem to be investigated is an elastic steel cylinder encased in a homogeneous, elastic, rock-like material subjected to a surface blast loading.

Within the above framework, the objectives of this study include:

(1) Identification and discussion of explicit and implicit algorithms, including considerations of numerical stability and accuracy.

(2) Comparison of efficiency between explicit and implicit for the test boundary value problem and estimates for a nonlinear case.

(3) Development of a combined explicit-implicit integration algorithm for superior efficiency.

Approach

It is recognized that an efficiency comparison of explicit versus implicit schemes (Objective 2) is relative and subjective. That is, the relative merits of the two integration schemes are not only dependent on the nature of the boundary value problem, but also on the programming skill of the program authors and the particular costing algorithm of the host computer site.

To minimize the influence of different programmers, the finite element program FEAP [9] was adopted for this study. FEAP is the only known general purpose finite element code containing both explicit and implicit algorithms based on the Newmark β-method. It is a linear code (also linear viscoelastic) with two- and three-dimensional elements.

With regard to the host computer site (CDC 6600), only central processing time will be considered for efficiency comparisons without regard to input/output (I/O) time. Although I/O time may be significant, particularly for out-of-core solution methods, it is not considered in this study because the associated costs are arbitrary and dependent on the costing algorithm of the operating site.

In the following pages, the Newmark β-method is reviewed in the context of explicit and implicit algorithms, together with a discussion of numerical stability and integration accuracy. Next, the FEAP code is used to ascertain the efficiency of explicit versus implicit for the stated test problem. Lastly, a combined explicit-implicit algorithm is presented followed by conclusions and recommendations.

THEORETICAL CONSIDERATIONS OF NEWMARK β-METHOD

For this investigation, we consider the spatially discretized matrix equation of structural dynamics given by:

$$\underline{\underline{M}}\,\ddot{\underline{u}} + \underline{\underline{K}}\,\underline{u} = \underline{f} \tag{1}$$

where: $\underline{\underline{M}}$ = mass matrix

$\underline{\underline{K}}$ = stiffness matrix

$\ddot{\underline{u}}$ = acceleration vector

$\dot{\underline{u}}$ = velocity vector

$\underline{u}$ = displacement vector

$\underline{f}$ = external load vector

Equation 1 is a coupled system of second-order ordinary differential equations which represents an initial-value problem for finding the displacement function $\underline{u}(t)$ satisfying Equation 1 and also satisfying the initial conditions $\underline{u}(0) = \underline{u}_o$ and $\dot{\underline{u}}(0) = \dot{\underline{u}}_o$, where $\underline{u}_o$ and $\dot{\underline{u}}_o$ are given initial data. The matrix $\underline{\underline{M}}$ is assumed constant, symmetric, and positive definite. The stiffness matrix $\underline{\underline{K}}$ is also assumed positive definite, but not necessarily constant, to reflect a changing stiffness due to material nonlinearity.

Newmark β-Method

A step-by-step operator suitable for numerically integrating Equation 1 is given by Newmark [3] as:

$$\dot{\underline{u}}_{t+\Delta t} = \dot{\underline{u}}_t + \Delta t[(1 - \gamma)\ddot{\underline{u}}_t + \gamma\ddot{\underline{u}}_{t+\Delta t}] \tag{2}$$

$$\underline{u}_{t+\Delta t} = \underline{u}_t + \Delta t\dot{\underline{u}}_t + \Delta t^2[(1/2 - \beta)\ddot{\underline{u}}_t + \beta\ddot{u}_{t+\Delta t}] \tag{3}$$

where: Δt = time step

β = Newmark β-parameter, $0 \lesssim \beta \lesssim 1/4$

γ = Newmark numerical damping parameter ($\gamma = 1/2$)

The damping parameter γ introduces numerical damping when $\gamma \neq 1/2$. In this study, γ is taken as 1/2 to avoid complications of numerical damping. Subscripts denote the time at which the response is evaluated.

Specification of the β-parameter ($\beta \neq 0$) leads to a variety of well-known implicit schemes. For example, $\beta = 1/4$ is equivalent to the average acceleration scheme, and $\beta = 1/6$ is equivalent to the linear acceleration scheme. For the special case $\beta = 0$, an explicit scheme results, as can be observed from Equation 3 wherein displacements at time $t + \Delta t$ are predicted from known responses at the previous time t.

Computational algorithms for implicit ($\beta \neq 0$) and explicit ($\beta = 0$) integrations are outlined in the next sections.

Implicit Algorithm

It is assumed the responses $\underline{u}_t$, $\dot{\underline{u}}_t$, and $\ddot{\underline{u}}_t$ are known for time t, and the objective is to determine these responses at time $t + \Delta t$. To this end, the following three steps constitute an implicit algorithm:

Step 1. From Equation 3, express $\ddot{\underline{u}}_{t+\Delta t}$ as a function of $u_{t+\Delta t}$ and previous responses to get:

$$\ddot{\underline{u}}_{t+\Delta t} = (1/\beta\Delta t^2)\underline{u}_{t+\Delta t} - \underline{a}_t$$

where: $$\underline{a}_t = \left(\frac{1}{\beta\Delta t^2}\right)\underline{u}_t + \left(\frac{1}{\beta\Delta t}\right)\dot{\underline{u}}_t + \left(\frac{1}{2\beta} - 1\right)\ddot{\underline{u}}_t$$

Step 2. Inserting the above expression for $\ddot{\underline{u}}_{t+\Delta t}$ into Equation 1, $\underline{u}_{t+\Delta t}$ is determined from the solution of the coupled system:

$$\left[\left(\frac{1}{\beta\Delta t^2}\right)\underline{M} + \underline{K}\right]\underline{u}_{t+\Delta t} = \underline{f}_{t+\Delta t} + \underline{M}\underline{a}_t$$

Step 3. Update accelerations using the expression in Step 1, and update velocities using Equation 2, i.e.,

$$\ddot{\underline{u}}_{t+\Delta t} = \left(\frac{1}{\beta\Delta t^2}\right)\underline{u}_{t+\Delta t} - \underline{a}_t$$

$$\dot{\underline{u}}_{t+\Delta t} = \dot{\underline{u}}_t + \frac{\Delta t}{2}(\ddot{\underline{u}}_t + \ddot{u}_{t+\Delta t})$$

The above algorithm is repeated successively for each time step through the time range of interest.

Step 2 of the above algorithm requires assembling the global mass and stiffness matrix and solving the coupled system by techniques such as elimination (i.e., triangularization), which is a costly operation. If the system is linear and a constant size time step is used, the triangularization can be done once and for all at the outset of the procedure so that subsequent steps only require modifying the right-hand side and performing back substitution. However, for nonlinear systems the stiffness matrix may have to be reformed and, hence, resolved at every time step and perhaps iterations within the time step, depending on the degree of nonlinearity and the methodology employed. This disadvantage of the implicit method is not shared by the explicit algorithm discussed next.

Explicit Algorithm

As before, it is assumed the responses $\underline{u}_t$, $\dot{\underline{u}}_t$, and $\ddot{\underline{u}}_t$ are known and the objective is to determine the responses at time $t + \Delta t$. The following three steps constitute an explicit algorithm.

Step 1. From Equation 3 with $\beta = 0$, the displacements $u_{t+\Delta t}$ are predicted directly as a function of the previous responses:

$$\underline{u}_{t+\Delta t} = \underline{d}_t$$

where: $$\underline{d}_t = \underline{u}_t + \Delta t \dot{\underline{u}}_t + \frac{\Delta t^2}{2} \ddot{\underline{u}}_t$$

Step 2. Inserting the above expression for $u_{t+\Delta t}$ into Equation 1, the accelerations $\ddot{u}_{t+\Delta t}$ are given by the solution of:

$$\underline{\underline{M}}\, \ddot{\underline{u}}_{t+\Delta t} = \underline{f}_{t+\Delta t} - \underline{\underline{K}}\, \underline{d}_t$$

Step 3. Lastly, the velocities $\dot{\underline{u}}_{t+\Delta t}$ are updated from Equation 2, i.e.:

$$\dot{\underline{u}}_{t+\Delta t} = \dot{\underline{u}}_t + \frac{\Delta t}{2} [\ddot{\underline{u}}_t + \ddot{\underline{u}}_{t+\Delta t}]$$

Unlike Step 2 of the implicit algorithm, Step 2 of the explicit algorithm only requires assembling the global mass matrix $\underline{\underline{M}}$. If the lumped mass technique is adopted, then $\underline{\underline{M}}$ is diagonal and the solution for $\ddot{\underline{u}}_{t+\Delta t}$ is trivial (otherwise $\underline{\underline{M}}$ must be triangularized once at the outset). Furthermore, the internal force vector represented by $\underline{\underline{K}}\underline{d}_t$ can be easily computed at the element level circumventing the need of formally assembling the global stiffness $\underline{\underline{K}}$. Accordingly, there is no significant penalty in the algorithm for nonlinear systems since changes in $\underline{\underline{K}}$ are easily accommodated by right-hand-side operations at the element level.

The apparent advantages of the explicit over implicit algorithm are mitigated by the concern of numerical stability which limits the size of the integration step Δt. These notions are discussed next.

Stability of Newmark β-Method

Numerical stability of a solution algorithm may generally be assured by proper choice of the integration step size. Since stability increases with decreasing step size, a sufficiently small step can generally be found to provide a stable solution. Therefore, the question to be explored is, what size time step is required for stability of the Newmark β-method. The following development is restricted to linear systems. Stability for nonlinear systems has been addressed on an energy basis [10, 11].

It is well-known that a linear system represented by Equation 1 can be transformed into an equivalent set of uncoupled equations through modal analysis. A typical uncoupled modal equation may be written as:

$$\ddot{X} + \omega^2 X = p(t) \tag{4}$$

where X is the transformed displacement called the normal coordinate, ω is the associated frequency of vibration, and p(t) is the transformed loading function.

It is asserted that the numerical integration of all the modal equations (typified by Equation 4) using the same Δt is equivalent to the numerical integration of the coupled system (Equation 1). Accordingly, numerical stability can be simplified to the investigation of Equation 4.

To this end, the Newmark integration operator (Equations 2 and 3) can be combined and expressed independently of velocities by taking the difference of Equation 3 at time t + Δt from its value at time t and replacing the resulting velocity difference by Equation 2. This gives:

$$X_{t+\Delta t} - 2X_t + X_{t-\Delta t} = \Delta t^2[\beta\ddot{X}_{t+\Delta t} + (1-2\beta)\ddot{X}_t + \beta\ddot{X}_{t-\Delta t}] \tag{5}$$

where the nodal displacement $\underline{u}$ is replaced by the normal coordinate X.

For the case of free vibration p(t) = 0, Equation 4 is introduced into the integration operator (Equation 5) at times t - Δt, t, and t + Δt, resulting in the difference scheme:

$$X_{t+\Delta t} - bX_t + X_{t-\Delta t} = 0 \tag{6}$$

where
$$b = \frac{2 - (\omega\Delta t)^2 (1 - 2\beta)}{1 + (\omega\Delta t)^2 \beta} \tag{7}$$

Equation 6 represents a step-by-step finite difference scheme for successively updating the displacements $X_{t+\Delta t}$ in terms of the previous displacements X_t and $X_{t-\Delta t}$.

For a given set of initial conditions, the free vibration of a linear system must be harmonic and bounded. Thus, the stability question is stated: for a particular β and maximum frequency ω_{max}, how large a time step, Δt, may be taken so that Equation 6 will produce bounded and harmonic results? This question is answered by determining the difference solution which is achieved by initially assuming a solution of the form:

$$X_{t_k} = r^{(t_k/\Delta t)} \tag{8}$$

where k is the time step counter $k = t_k/\Delta t$, and r is to be determined. Inserting the above into Equation 6 leads to the characteristic equation for r:

$$r^2 - br + 1 = 0 \tag{9}$$

whose roots r_1, r_2 in complex polar form are:

$$r_1, r_2 = e^{\pm iq} \tag{10}$$

where
$$q = \sin^{-1}\left(\sqrt{1 - b^2/4}\right) \tag{11}$$

Since $e^{iqt_k/\Delta t} = \cos(qt_k/\Delta t) + i \sin(qt_k/\Delta t)$, the difference solution of Equation 6 may be written in the form:

$$X_{t_k} = A \cos\left(\frac{qt_k}{\Delta t}\right) + B \sin\left(\frac{qt_k}{\Delta t}\right) \tag{12}$$

where A and B are real constants determined from initial conditions; $A = X(0)$, $B = (\Delta t/q)\,\dot{X}(0)$. The above equation yields a bounded, harmonic solution for X_{t_k}, providing q is real. Clearly, from Equation 11, q is real if $(1 - b^2/4) \geq 0$. This provides the stability criterion, such that replacing b with Equation 7, the maximum allowable time step is given by:

$$\Delta t \leq \frac{T}{2\pi}\sqrt{\frac{4}{1 - 4\beta}} \tag{13}$$

where T is the shortest period of vibration of the system given by $T = 2\pi/\omega_{max}$.

Evaluating Equation 13, the allowable time step for the explicit case, $\beta = 0$, is $\Delta t \leq 0.318$ T. For implicit examples, $\beta = 1/6$ gives $\Delta t \leq 0.551$ T, but for $\beta = 1/4$ there is no finite limit on Δt for stability. Hence, $\beta = 1/4$ provides an unconditionally stable operator.

For all cases $\beta < 1/4$, the allowable time step to insure stability is dependent on the shortest period of the system as given by Equation 13. Unfortunately, the value of the shortest period (or highest frequency) is generally not known and troublesome to calculate. As an alternative, it is often more convenient to determine the stability limit of Δt by a heuristic approach given next.

Heuristic Stability Criterion

In lieu of using Equation 13 for selecting a stable time step, the following relationship may be used:

$$\Delta t \leq (h/c)_{min} \sqrt{1/(1 - 4\beta)} \quad (14)$$

where h is the shortest side of a finite element, c is the maximum wavespeed of the element material, and $(h/c)_{min}$ implies the controlling element in the mesh where the ratio h/c is a minimum. (For isotropic elastic materials, the maximum wavespeed is $c = \{E(1-\nu)/[\rho(1+\nu)(1-2\nu)]\}^{1/2}$, where E = Young's Modulus, ν = Poisson's ratio, and ρ = mass density.)

The genesis of Equation 14 is based on heuristic arguments for the explicit algorithm ($\beta = 0$) and modified by the factor $\sqrt{1/(1 - 4\beta)}$ for implicit cases as discussed in the following.

Consider the continuum body shown in Figure 1 with an arbitrary finite element topology drawn on the body and focus attention on the node common to the four shaded elements. If this point is perturbed by an external agency, continuum theory requires the excitation to travel with a sonic wavespeed c. Therefore, after a time interval, Δt, the perturbed area is inscribed by a circle of radius $r_c = c\Delta t$, shown by the dashed line in Figure 1. Now, for the corresponding explicit algorithm, the perturbed area for one time step can be no greater than the area of numerical coupling; i.e., the internal forces $\underline{K}\underline{d}$ generated by an excitation of the common node during one time step are coupled no further than the nodes of the shaded elements. This condition holds for each and every node as it, in turn, becomes excited. Therefore, in order to insure that the ''numerical wavespeed'' of the explicit algorithm can excite an area at least as large as the area of sonic travel, it is required that $h \geq r_c$ or, equivalently, $\Delta t \leq (h/c)_{min}$.

With regard to the implicit algorithm $\beta \neq 0$, the numerical coupling is greater because we are, in effect, operating with $\underline{K}^{-1}$ and not the banded matrix $\underline{K}$. Since $\underline{K}^{-1}$ is generally fully populated (although weakly coupled between distant nodes), the area of numerical coupling is effectively greater. Accordingly, the maximum allowable time step is increased by the factor $\sqrt{1/(1 - 4\beta)}$, which is the ratio from Equation 13: $\Delta t(\beta \neq 0) \div \Delta t(\beta = 0)$.

Experience has shown that Equation 14 provides a good estimate of an allowable time step for stability.

Accuracy of Newmark β-Method

The selection of Δt to insure numerical stability is a necessary condition for a meaningful solution; however, it is not automatically a sufficient condition to insure that the numerical results are a good approximation of the original differential equation. This becomes the question of accuracy. An obvious example is the case $\beta = 1/4$ which has no stability limit for Δt so that Δt is controlled strictly from accuracy considerations.

Accuracy can be studied by comparing the exact solution of the original differential equation (Equation 4) with the corresponding difference solution given by Equation 12. Specifically, for the case of

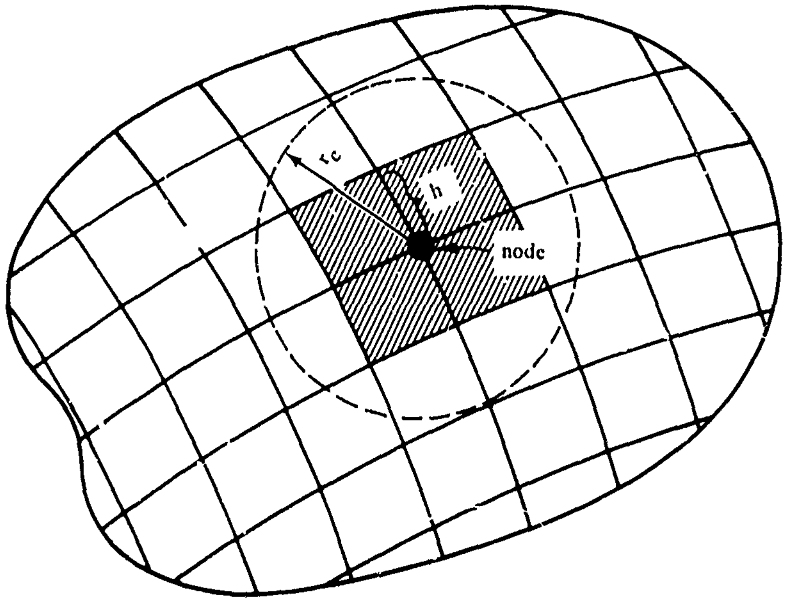


Figure 1. Representation of numerical and continuum wavespeed.

free vibration, the exact solution has the form $X = A\cos\omega t + B\sin\omega t$, whereas Equation 12 has the form $X_{t_k} = A\cos\bar{\omega}t_k + B\sin\bar{\omega}t_k$, where $\bar{\omega} = q/\Delta t$. For harmonic similarity, the numerical frequency $\bar{\omega}$ must be a good approximation of the actual frequency ω; or, equivalently, the numerical period $\bar{T} = 2\pi/\bar{\omega}$ must be a good approximation of the actual period $T = 2\pi/\omega$.

The ratio of the approximate period to the actual period provides a measure of accuracy [12]. With the aid of Equation 11, this ratio may be written as:

$$\frac{\bar{T}}{T} = \frac{2\pi\,(\Delta t/T)}{\sin^{-1}\left(\sqrt{1 - b^2/4}\right)} \tag{15}$$

where

$$b = \frac{2 - \left(2\pi\,\frac{\Delta t}{T}\right)^2 (1-2\beta)}{1 + \left(2\pi\,\frac{\Delta t}{T}\right)^2 \beta} \tag{16}$$

As $\Delta t \to 0$, $\bar{T}/T \to 1$, illustrating that the approximate solution approaches the exact solution in the limit. However, for increasing values of Δt, $\bar{T}/T$ diverges from unity on a path dependent on β. Figure 2 illustrates this trend for $\beta = 0$, 1/6, and 1/4 as a function of $\Delta t/T$. It is observed that $\bar{T}/T$ begins to significantly deviate from unity when $\Delta t/T$ is larger than say 0.2, which is smaller than the stability limits.

From the above observations, it would appear that accuracy considerations place a more stringent limit on the maximum time step than does the stability criterion. However, this is generally not true for multi-degree-of-freedom systems typical of finite element models. The reason for this is that the vibration modes associated with higher frequencies (shorter periods) generally have very low participation factors. Thus, even though the higher modes may be integrated with significant error, their net contribution is masked by the large participation factors of the dominant lower modes whose integration is more accurate due to the longer periods. Also, it is known that the higher vibration modes of a finite element model are ''fictitious'' in the sense that they represent a lumping of the infinite set of higher modes of vibration corresponding to the continuous system being modeled. Therefore, the low participation of the fictitious vibration modes is not merely a fortuitous happenstance, but rather is a necessary consequence of proper spatial discretization.

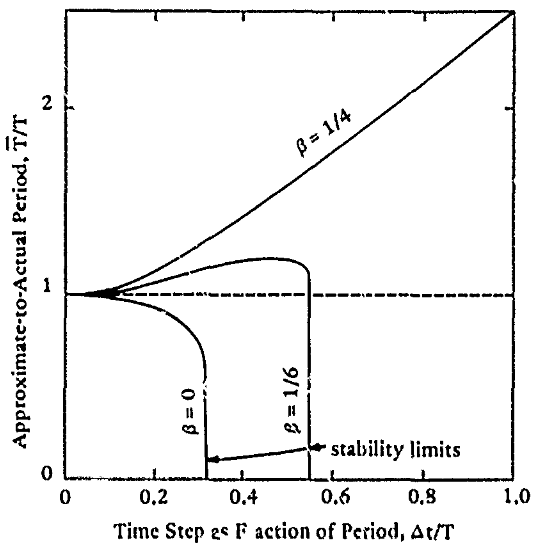


Figure 2. Period accuracy of Newmark β-method.

To summarize, for the cases $\beta < 1/4$ the allowable time step is generally governed by the stability criterion (Equation 13 or 14) based on the shortest period. Unlike the accuracy consideration, the shortest period (highest mode) cannot be ignored because, even though it initially has a low participation factor, if it is integrated in the unstable range, its contribution will grow without bound.

For the unconditionally stable case $\beta = 1/4$, the allowable time step is governed strictly by accuracy considerations. Since the analyst may have no idea of the frequency content of the mesh nor what frequencies will be dominant for a specified loading, it is difficult to determine a priori an optimum time step size. Accordingly, computational experimentation is generally the most direct method. As a guide, the time step should be at least sufficiently small to define the shape and character of the loading function.

In the next section computational experimentation is performed on the test problem posed in the objective of this report.

COMPUTATIONAL INVESTIGATION

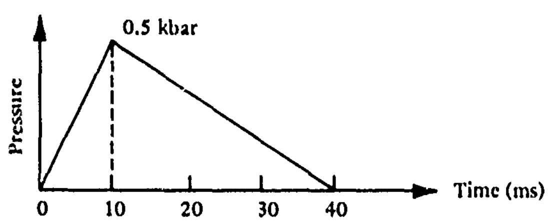
The finite element code FEAP [9] is used to study the efficiency of the implicit algorithm $\beta = 1/4$ versus the explicit algorithm $\beta = 0$. FEAP's explicit and implicit algorithms accept identical finite element

input records and use the same element stiffness routine. Thus, it may be presumed the subsequent comparisons provide an unbiased assessment of integration efficiency.

The test problem described is representative of a class of problems of current interest to DNA [1, 2].

Test Problem and Finite Element Model

The test problem is illustrated in Figure 3 which shows a system composed of a homogeneous media representative of a soft rock-like material called tuff and a 3-foot (0.914 m) circular steel liner 0.78 inch (1.98 cm) thick. All materials are elastic and are defined in Figure 3. Plane strain geometry is assumed, and the system is symmetric about the vertical centerline.



Material	Young's Modulus (psi x 10^6)	Poisson's Ratio	Mass Density (slug-ft/in.^{4})	Wavespeed (in./ms)
Tuff	0.448	0.286	0.00018	57.0
Steel	30.0	0.30	0.00073	235.0

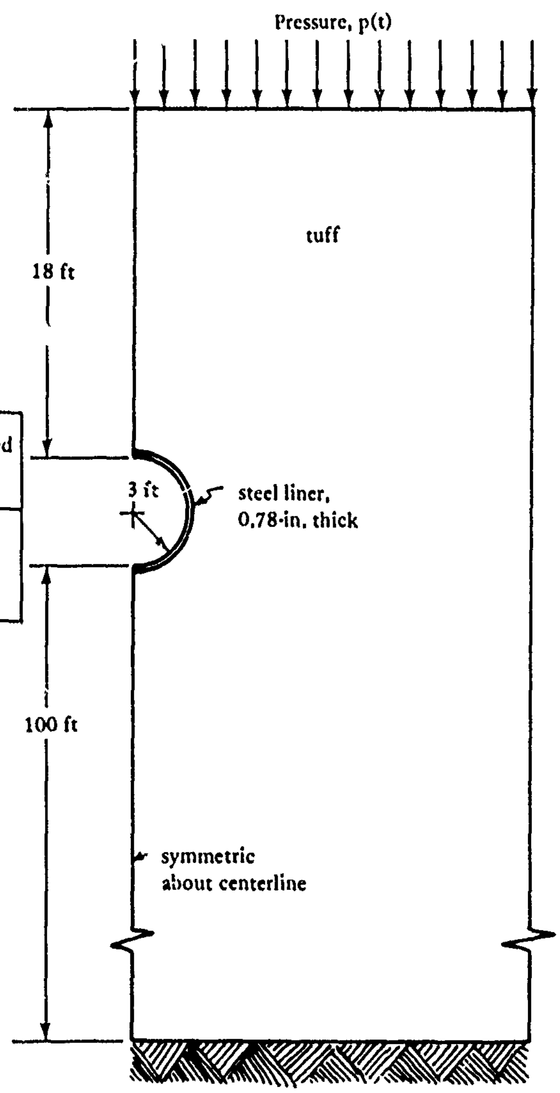


Figure 3. Test problem, loading, and material properties.

Pressure loading is distributed uniformly along the surface of the tuff, and the loading function is a triangular pulse whose rise time is 10 ms with a maximum pressure of 0.5 kbar followed by a 30-ms decay to zero pressure.

The finite element mesh topology representing the test problem is shown in Figure 4. All elements are compatible four-node, isoparametric elements. The steel liner is coarsely modeled with a single layer of 32 elements forming a semicircle. Although the single layer is insufficient to accurately capture bending of the liner, it suffices for this investigation where the concern is with time integration.

A simple lumped-mass procedure is used for both explicit and implicit integration schemes. Boundary conditions, degrees of freedom, average bandwidth, and other information are displayed in Figure 4.

Explicit Results ($\beta = 0$)

Solutions were attempted for time steps of $\Delta t = 0.0025$, 0.0035, and 0.0045 ms. The solutions for $\Delta t = 0.0025$ and 0.0035 ms were practically identical, indicating these solutions provided accurate time integrations. A typical result is shown by the solid line in Figure 5, which is a normalized time-history plot of the thrust stress (i.e., average hoop stress) in the steel liner at the springline.

For the case $\Delta t = 0.0045$ ms, the responses in the steel liner became unstable (wildly erratic) after approximately 150 time steps or 0.68 ms. Thereafter, instability quickly spread throughout the entire system in a matter of a few time

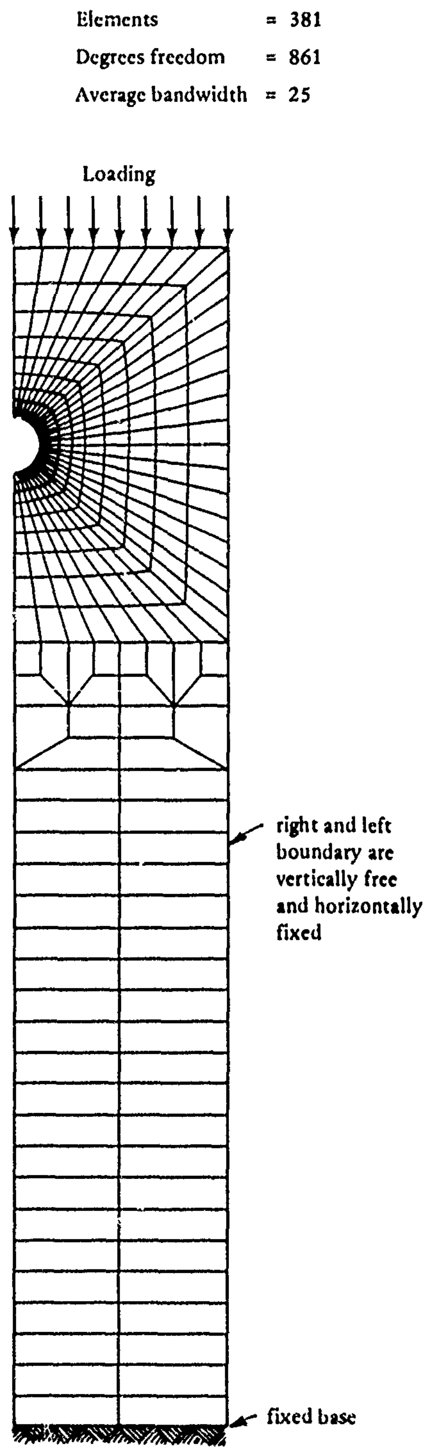


Figure 4. Finite element mesh of test problem.

steps. Theoretically, the sonic travel time for a surface disturbance to travel through 18 feet (5.49 m) of tuff and excite the liner is 3.8 ms. However, the numerical wave speed can travel vertically downward one element depth per time step and prematurely excite the instability of the steel liner well ahead of the sonic travel time.

The heuristic stability prediction for maximum allowable Δt (Equation 14) based on the steel liner elements is $\Delta t = 0.0033$ ms [i.e., h = 0.78 inch (1.98 cm), c = 235 in./ms (597 cm/ms)]. This is in good agreement with the observed instability occurring between $0.0035 < \Delta t < 0.0045$ ms. Computer time for the central processor is summarized in Table 1.

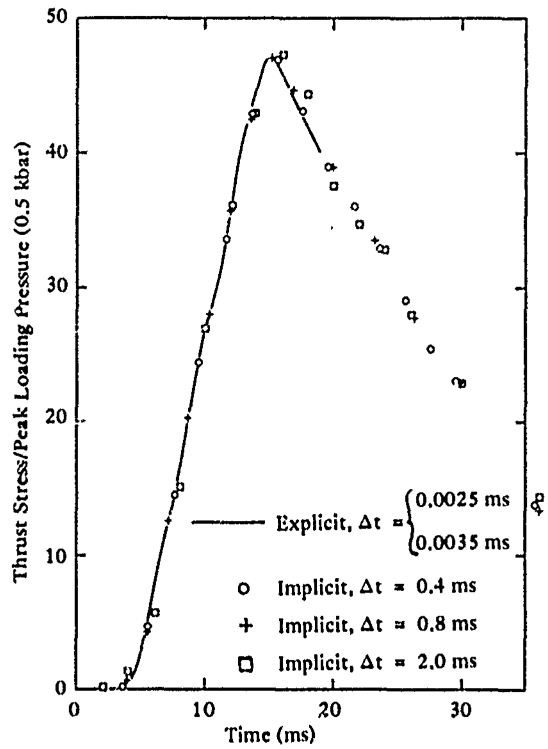


Figure 5. History plots of steel liner thrust stress, implicit and explicit.

Implicit Results ($\beta = 1/4$)

Solutions were obtained for the time steps $\Delta t = 0.4$, 0.8, and 2.0 ms, which are two orders of magnitude greater than the allowable explicit time steps. Since $\beta = 1/4$ provides an unconditionally stable implicit algorithm, the only concern is with accuracy. In each case, the results were in close agreement with each other and the explicit solution as illustrated by the discrete symbols superimposed on the explicit solution presented in Figure 5. A slight error can be observed near the peak of the response for the case $\Delta t = 2.0$ ms. Accordingly, for the sake of subsequent comparisons, it will be said that the maximum allowable time step based on accuracy is $\Delta t = 0.8$ ms. This corresponds to 12 time steps within the loading rise time. Computer cost (time) for the central processor is summarized in Table 1.

Efficiency of Explicit Versus Implicit

The computer times reported in Table 1 were determined by assessing a system ''clock routine,'' which measures the actual running time of each step for both the explicit and implicit algorithms. These results indicate the number of time steps required to complete the 40 ms loading duration is 11500 (i.e., 40/0.0035) for the explicit case, but only 50 (i.e., 40/0.8) for the implicit case; or a ratio of 230 in favor of the implicit method. On the other hand, the computer cost (time) per step of

Table 1. Central Processor Time for Explicit and Implicit Algorithms

Algorithm	Computer Time Per Step of Algorithm (s)	Computer Time Per Complete Solution[a] (s)
Explicit ($\beta = 0$)	0.164	1,370.0
Implicit ($\beta = 1/4$)	4.23[b] or 1.22[c]	64.0

[a]Complete solution time is based on 40 ms problem, using $\Delta t = 0.0035$ ms for explicit and $\Delta t = 0.8$ ms for implicit.

[b]Time for a solution step requiring triangularization.

[c]Time for a solution step not requiring triangularization.

the implicit method, where the stiffness matrix is triangularized, is 25 times more than an explicit step cost. For subsequent steps not requiring triangularization, the implicit cost is 8 times more than the explicit cost per step. As a net result the computer cost (based on central processing time) of the explicit solution is 30 times more expensive than the implicit solution for a complete 40-ms run.

The observed efficiency of the implicit method is primarily due to the linear nature of the test problem.

Nonlinear systems do not appreciably alter the computer costs for explicit algorithms because stiffness changes are dealt with at the element level on the right-hand side of the equilibrium equations. Moreover, since the explicit step size is inherently small, iterations within the time step are generally not required. Conversely, nonlinear stiffnesses in the implicit method may require triangularizing and iterating within every time step, as well as reducing the size of the time step. For example, previous experience indicates that, if the tuff material is modeled with a nonhardening plasticity law, then to maintain accuracy for the implicit algorithm requires $\Delta t \approx 0.2$ ms, as well as triangularizing and iterating within each time step. Under these conditions, the computer cost can be estimated from Table 1 to be about equivalent to the cost of the explicit method.

Summarizing for the class of problems considered, the implicit algorithm is significantly more efficient for linear systems; however, for nonlinear systems the two methods are competitive. The most promising efficient scheme is a combined explicit/implicit algorithm (presented next).

COMBINING EXPLICIT AND IMPLICIT

The nature of the foregoing boundary value problem provides an illustrative example of the potential advantages of combining the explicit and implicit methods into a single algorithm. To see this, consider the advantages of applying the implicit algorithm to nodes (degrees of freedom) associated with the steel liner, while the remaining nodes (degrees of freedom) in the tuff are integrated with an explicit algorithm. With this assignment, explicit stability is governed by the larger and sonically slower tuff elements, resulting in a stable time step on the order of 10 to 100 times larger than the time step required when the steel elements govern. By the same token, the implicit algorithm is significantly enhanced because only the small portion of the stiffness matrix associated with the steel liner needs triangularization.

The above concepts are presented more formally in the following general discussion. Consider an arbitrary body discretized by finite elements such that all ''i'' nodes are to be integrated implicitly and all ''e'' nodes are to be integrated explicitly. These nodes are denoted in Figure 6 by a dashed line encompassing the ''i'' nodes, and all nodes exterior to the dashed curve are ''e'' nodes. Those element stiffnesses associated with only ''i'' nodes are denoted by $\underline{K}_{ii}$, while those associated with only ''e'' nodes are expressed as $\underline{K}_{ee}$. Mixed elements associated with both ''e'' and ''i'' nodes are denoted by $\underline{K}_{ei}$.

With these definitions, the equilibrium equation (Equation 1) can be written in partitioned form as:

$$\begin{bmatrix} M_e & \\ & M_i \end{bmatrix} \begin{Bmatrix} \ddot{u}_e \\ \hline \ddot{u}_i \end{Bmatrix} + \left[\begin{array}{c|c} K_{ee} & K_{ei} \\ \hline K_{ie} & K_{ii} \end{array}\right] \begin{Bmatrix} u_e \\ \hline u_i \end{Bmatrix} = \begin{Bmatrix} f_e \\ \hline f_i \end{Bmatrix} \tag{17}$$

where u_e, u_i = displacements at explicit, implicit nodes

$\ddot{u}_e$, $\ddot{u}_i$ = accelerations at explicit, implicit nodes

M_e, M_i = lumped masses at explicit, implicit nodes

f_e, f_i = nodal forces at explicit, implicit nodes

K_{ee} = global stiffness of elements with only ''e'' nodes

K_{ii} = global stiffness of elements with only ''i'' nodes

K_{ei} = K_{ie}^T = global stiffness of elements with both e and i nodes

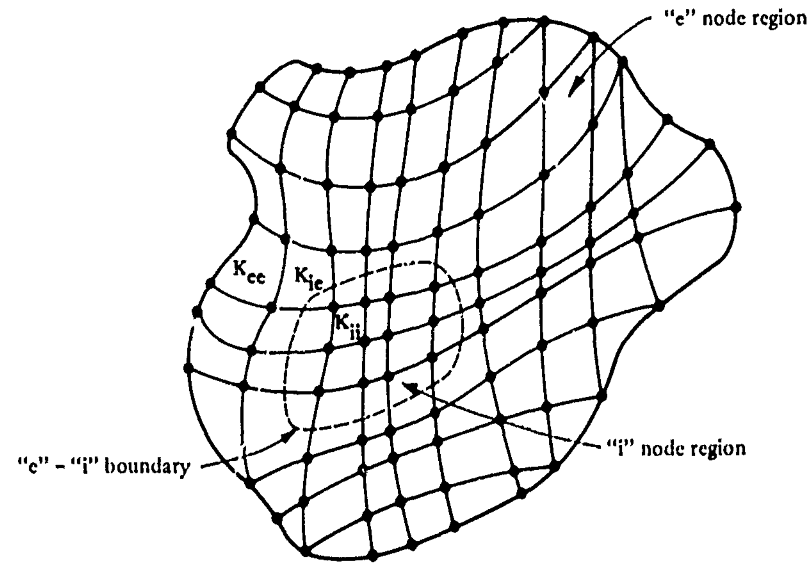


Figure 6. Conceptualization of explicit and implicit integration regions.

Expressing the partitioned equilibrium equation as two coupled systems of equations gives

$$[M_e]\ \{\ddot{u}_e\} + [K_{ee}]\ \{u_e\} + [K_{ei}]\ \{u_i\} = \{f_e\} \qquad (18)$$

$$[M_i]\ \{\ddot{u}_i\} + [K_{ii}]\ \{u_i\} + [K_{ie}]\ \{u_e\} = \{f_i\} \qquad (19)$$

To numerically integrate Equations 18 and 19 step-by-step, it is assumed the responses $\{u_e\}_t$, $\{u_i\}_t$ and their first two derivatives are known for time t, and the objective is to determine the responses $\{u_e\}_{t+\Delta t}$, $\{u_i\}_{t+\Delta t}$ and their first two derivatives for time t + Δt. To this end, the following procedure constitutes a combined explicit-implicit algorithm using the Newmark β-method defined by Equations 2 and 3.

Step 1. Predict the ''e'' nodal displacements $\{u_e\}_{t+\Delta t}$ directly from Equation 3 with $\beta = 0$, (i.e., explicit) to get:

$$\{u_e\}_{t+\Delta t} = \{d_e\}_t$$

where $$\{d_e\}_t = \{u_e\}_t + \Delta t\{\dot{u}_e\}_t + \frac{\Delta t^2}{2}\{\ddot{u}_e\}_t$$

Step 2. Again using Equation 3 with $\beta \neq 0$, express $\{\ddot{u}_i\}_{t+\Delta t}$ as a function of $\{u_i\}_{t+\Delta t}$ and previous responses to get:

$$\{\ddot{u}_i\}_{t+\Delta t} = \left(\frac{1}{\beta \Delta t^2}\right) \{u_i\}_{t+\Delta t} - \{a_i\}_t$$

where $$\{a_i\}_t = \left[\left(\frac{1}{\beta \Delta t^2}\right) \{u_i\}_t + \left(\frac{1}{\beta \Delta t}\right)\{\dot{u}_i\}_t + \left(\frac{1}{2\beta} - 1\right) \{\ddot{u}_i\}_t\right]$$

Step 3. Inserting the above expression for $\{\ddot{u}_i\}_{t+\Delta t}$ into Equation 19, $\{u_i\}_{t+\Delta t}$ is determined by solving the coupled system:

$$\left[\left(\frac{1}{\beta \Delta t^2}\right) [M_i] + [K_{ii}]\right]\{u_i\}_{t+\Delta t} = \{f_i\}_{t+\Delta t} - [K_{ie}]\{u_e\}_{t+\Delta t}$$

$$+ [M_i] \{a_i\}_t$$

Step 4. Having determined $\{u_e\}_{t+\Delta t}$ and $\{u_i\}_{t+\Delta t}$, compute the corresponding accelerations using Equation 18 for $\{\ddot{u}_e\}_{t+\Delta t}$ and the first equation in Step 2 for $\{\ddot{u}_i\}_{t+\Delta t}$ to get:

$$\{\ddot{u}_e\}_{t+\Delta t} = [M_e]^{-1} (\{f_e\}_{t+\Delta t} - [K_{ee}] \{u_e\}_{t+\Delta t} - [K_{ei}] \{u_i\}_{t+\Delta t})$$

$$\{\ddot{u}_i\}_{t+\Delta t} = \left(\frac{1}{\beta \Delta t^2}\right) \{u_i\}_{t+\Delta t} - \{a_i\}_t$$

Step 5. Lastly, update the velocities using Newmark's expression, Equation 2

$$\left\{\begin{array}{c}\dot{u}_e \\ \hline \dot{u}_i\end{array}\right\}_{t+\Delta t} = \left\{\begin{array}{c}\dot{u}_e \\ \hline \dot{u}_i\end{array}\right\}_t + \frac{\Delta t}{2}\left(\left\{\begin{array}{c}\ddot{u}_e \\ \hline \ddot{u}_i\end{array}\right\}_t + \left\{\begin{array}{c}\ddot{u}_e \\ \hline \ddot{u}_i\end{array}\right\}_{t+\Delta t}\right)$$

This procedure is repeated step-by-step throughout the time of interest.

The advantages of the combined explicit-implicit algorithm is quite remarkable in that it is potentially one or two orders of magnitude more efficient than either method applied individually. Note that the only triangularization required is in Step 3 for the submatrix $[K_{ii}]$ whose size is small compared to the entire system (e.g., steel elements). Moreover, the average bandwidth of $[K_{ii}]$ is easily minimized by judicious compact node numbering of the ''i'' nodes, which implies rapid solutions with minimal storage. Node numbering of ''e'' nodes has no bearing on the solution efficiency since all stiffness operations involving ''e'' nodes are matrix multiplications performed at the element level. Since the domain of the ''e'' nodes are selected to permit the explicit stability criterion to be based on the larger and sonically slower elements, the critical time step may be increased by one or two orders of magnitude, depending on the nature of the problem.

It is easy to conceive of large, three-dimensional, nonlinear problems such that a combined method as presented here may be the only economically feasible alternative of obtaining a solution. Hence, combined methods should be vigorously investigated.

CONCLUSIONS AND RECOMMENDATIONS

Within the class of problems and limitations defined in this study, the following comments appear valid for numerical integration by the Newmark β-method.

1. The maximum allowable time step for conditionally stable schemes ($\beta < 1/4$) is generally controlled by the stability criterion, Equation 13 or 14.

2. The maximum allowable time step for the unconditionally stable scheme ($\beta = 1/4$) is controlled by accuracy considerations which may be determined by computational experimentation. As a guide, define the time step to subdivide the rise time into 10 increments.

3. For the linear system studied and computer/program employed, the implicit algorithm ($\beta = 1/4$) allows a time step more than 200 times larger than the explicit method ($\beta = 0$) with equivalent accuracy. However, each step of the implicit algorithm is 8 to 25 times more costly in computer time than a step of the explicit algorithm depending on whether or not triangularization is required. As a net result the implicit method was approximately 30 times more efficient.

4. Nonlinear systems penalize implicit algorithms much more severely than explicit algorithms to the extent that the two methods become equally competitive for the class of problems considered.

5. The combined explicit/implicit algorithm has the potential of enhancing efficiency by one or more orders of magnitude. It is recommended that combined integration methods be thoroughly investigated.

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